Ideal Gas Mixtures

Each constituent of a mixture is referred to as a species.

An ideal gas mixture, at temperature T_m, in a container of volume $\forall_m$ has the following characteristics:

$p_m = p_1 + p_2 + \cdots + p_n$ [1, 2, ..., n represent the species]

$T_m = T_1 = T_2 = \cdots = T_n$

$\forall_m = \forall_1 = \forall_2 = \cdots = \forall_n$ see Eqn (2.23), p 38

$H_m = H_1 + H_2 + \cdots + H_n$

$S_m = S_1 + S_2 + \cdots + S_n$

Consider the equation of state for each species

$p_1 \forall_m = n_1 \bar{R} T_m$ [n_1 - # of kmol of species 1, p_1 is the partial pressure of species 1]

$p_2 \forall_m = n_2 \bar{R} T_m$ [partial pressure of a species is the pressure exerted by it while occupying the container all by itself at the mixture pressure]

$\vdots \qquad \vdots$

$p_n \forall_m \bar{R} T_m$

Add: $\underbrace{(p_1 + p_2 + \cdots + p_n)}_{\text{This is the mixture pressure } p_m} \forall_m = \underbrace{(n_1 + n_2 + \cdots + n_n)}_{} \bar{R} T_m$

(n_m - total number of moles in the mixture)

The equation of state for the mixture is

$$\boxed{p_m \forall_m = n_m \bar{R} T_m}$$

The equation of state for species i is

$$p_i \forall_m = n_i \bar{R} T_m$$

$$\Rightarrow \frac{p_i}{p_m} = \frac{n_i}{n_m} \qquad \{\text{see Eqn } (2.25)\}$$

The mole fraction of species i is defined as

$$\boxed{X_i \stackrel{\text{def}}{=} \frac{n_i}{n_m}} \qquad \text{Eqn } (2.26)$$

$$\Rightarrow \boxed{\frac{p_i}{p_m} = X_i}$$

<u>Mass-specific Properties:</u>

$$h_i, \; s_i, \; c_{pi}, \; c_{vi}, \; R_i$$

<u>Mole-specific Properties</u>

$$\bar{h}_i, \; \bar{s}_i, \; \bar{c}_{pi}, \; \bar{c}_{vi}, \; \bar{R}$$

Each kmol has mass equal to $\bar{M}$ kg. Therefore,

$$\bar{h}_i = \bar{M}_i h_i, \quad \bar{s}_i = \bar{M}_i s_i, \quad \bar{c}_{p_i} = \bar{M}_i c_{p_i}, \quad \bar{c}_{v_i} = \bar{M} c_{v_i}$$

$$\gamma_i = \frac{c_{p_i}}{c_{v_i}} = \frac{\bar{c}_{p_i}/\bar{M}_i}{\bar{c}_{v_i}/\bar{M}_i} = \frac{\bar{c}_{p_i}}{\bar{c}_{v_i}}$$

Consider $H_m = H_1 + H_2 + \cdots + H_n$

$$= n_1 \bar{h}_1 + n_2 \bar{h}_2 + \cdots + n_n \bar{h}_n$$

$$\bar{h}_m = \frac{H_m}{n_m} = \frac{n_1}{n_m} \bar{h}_1 + \frac{n_2}{n_m} \bar{h}_2 + \cdots + \frac{n_n}{n_m} \bar{h}_n$$

$$= X_1 \bar{h}_1 + X_2 \bar{h}_2 + \cdots + X_n \bar{h}_n$$

(or) $$\bar{h}_m = \sum_{i=1}^{n} (X_i \bar{h}_i)$$

Similarly, $\bar{s}_m = \sum_{i=1}^{n} (X_i \bar{s}_i)$, $\bar{c}_{p_m} = \sum_{i=1}^{n} (X_i \bar{c}_{p_i})$,

$$\bar{c}_{v_m} = \sum_{i=1}^{n} (X_i \bar{c}_{v_i}), \quad \bar{M}_m = \sum_{i=1}^{n} (X_i \bar{M}_i)$$

$$\gamma_m = \frac{\bar{c}_{p_m}}{\bar{c}_{v_m}}$$

Since all gases have the same universal gas constant, it is quicker to get γ_m from

$$\gamma_m = \frac{\bar{c}_{p_m}}{\bar{c}_{p_m} - \bar{R}}$$

Ex

The ideal gas product mixture formed by the combustion of H_2 and O_2 has the following characteristics:

species ($\bar{M}$)	# mol (kmol)	$\bar{c}_p \left(\frac{kJ}{kmol.K}\right)$	$\bar{h} \left(\frac{kJ}{kmol}\right)$	calculated X
O_2 (32)	0.1008	36.3	116233	0.0433
H_2 (2)	0.3170	32.9	105346	0.1363
O (16)	0.054	20.9	312065	0.0232
H (1)	0.109	20.9	283015	0.0469
OH (17)	0.233	33.5	149137	0.1002
H_2O (18)	1.512	48.27	−87266	0.6501

Calculate the total number of moles in the mixture, the species mole fractions, the mixture specific gas constant, and its molar-specific and mass-specific enthalpies. Also find the specific heat ratio of the mixture.

$$n_m = \sum n_i = 2.3258, \quad X_i = \frac{n_i}{n_m}, \text{ see table}$$

$$\bar{M}_m = \sum_{i=1}^{n} (x_i \bar{M}_i) = 15.48 \frac{kg}{kmol}$$

$$R_m = \frac{\bar{R}}{\bar{M}_m} = \frac{8314.3}{15.48} = 537 \frac{J}{kg\text{-}K}$$

$$h_m = \sum_{i=1}^{n} (X_i \bar{h}_i) = -1883 \frac{kJ}{kmol}$$

$$h_m = \frac{\bar{h}_m}{\bar{M}_m} = \frac{-1883}{15.48} = -121.7 \frac{kJ}{kg}$$

$$\bar{c}_{pm} = \sum_{i=1}^{n} X_i \bar{c}_{pi} = 42.258 \frac{kJ}{kmol\text{-}K}$$

$$\gamma_m = \frac{\bar{c}_{pm}}{\bar{c}_{pm} - \bar{R}} = \frac{42258}{42258 - 8314.3} = 1.24$$

If $\bar{c}_{pi}$ values are not given, the following may be assumed for a preliminary calculation.

$$\gamma_{mon} = 1.67, \quad \gamma_{di} = 1.29, \quad \gamma_{tri} = 1.17$$

In this case, get $\bar{c}_{pi}$ from $\bar{c}_{pi} = \frac{\gamma_i \bar{R}}{\gamma_i - 1}$. Then get $\bar{c}_{pm} = \sum_{i=1}^{n} X_i \bar{c}_{pi}$, and $\gamma_m = \frac{\bar{c}_{pm}}{\bar{c}_{pm} - \bar{R}}$

Ex: Reconsider previous problem. Calculate γ_m using the γ- approximations for the species.

$$\bar{c}_{p_i} = \frac{\gamma_i \bar{R}}{\gamma_i - 1}$$

$$\bar{c}_{p_{O_2}} = \bar{c}_{p_{H_2}} = \bar{c}_{p_{OH}} = \frac{\gamma_{di} \bar{R}}{\gamma_{di} - 1} = \frac{1.29 \bar{R}}{1.29 - 1} = 4.448 \bar{R}$$

$$\bar{c}_{p_O} = \bar{c}_{p_H} = \frac{\gamma_{mon} \bar{R}}{\gamma_{mon} - 1} = \frac{1.67 \bar{R}}{1.67 - 1} = 2.493 \bar{R}$$

$$\bar{c}_{p_{H_2O}} = \frac{\gamma_{tri} \bar{R}}{\gamma_{tri} - 1} = \frac{1.17 \bar{R}}{1.17 - 1} = 6.882 \bar{R}$$

$$\bar{c}_{pm} = \sum_{i=1}^{n} (X_i \bar{c}_{pi}) = 5.893 \bar{R}$$

$$\gamma_m = \frac{\bar{c}_{pm}}{\bar{c}_{pm} - \bar{R}} = \frac{5.893 \bar{R}}{5.893 \bar{R} - \bar{R}} = \frac{5.893 \bar{R}}{4.893 \bar{R}} = 1.20$$